REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	May 23, 1996	Final Tech. 12-1-94 -- 11-30-95

4. TITLE AND SUBTITLE

Molecular Spectra and Dynamics at Interfaces

5. FUNDING NUMBERS

Grant N00014-93-0122

6. AUTHOR(S)

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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Office of Naval Research

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

RET Code 4131072

11. SUPPLEMENTARY NOTES

This report coversthe period of final no-cost extension.

12a. DISTRIBUTION/AVAILABILITY STATEMENT

Unlimited

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

Treatment of the simultaneous dynamics of electrons and nuclei with full account of electron nuclear coupling has been applied to polymeric chains. Only the highest frequency longitudinal and transverse vibrational modes couples strongly to the electrons.

The quantum dynamics of electron transfer at metal surfaces and of the dissociation of diatomic adsorbates have been investigated to construct models of bonding and dynamics at surfaces, and to calculate rates of ion neutralization, and photodesorption times. Electronic charge transfer, leading to ion neutralization, was studied for the system Na^+ + W(110)

A method has been developed to treat the coupling of the very different time scales present in molecular dynamics for nuclear (slow) and electronic (fast) motions; it has been based on density operators in Liouville space.

The photodissociation of CO adsorbed on the Ni(001) surface by visible and UV light has been described using wavepacket dynamics for two coupled potential energy surfaces, including the vibrational degree of freedom of CO. The treatment incorporates dissipation and force fluctuations at the metal surface, within the diabatic electronic representation. Calculations show that dissipation by electron-hole excitation is a dominant mechanism.

14. SUBJECT TERMS	15. NUMBER OF PAGES
Computational Methods, Spectra, Dynamics, Molecular Collisions, Intermolecular Forces	4
	16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	UL

OFFICE OF NAVAL RESEARCH

GRANT OR CONTRACT N00014-93-1-0122

FINAL TECHNICAL REPORT, 12/1/94-11/30/95

R&T CODE 4131072

MOLECULAR SPECTRA AND DYNAMICS AT INTERFACES

PI'S: N. Yngve Öhrn and David A. Micha

Quantum Theory Project
WM 363, University of Florida
Gainesville, FL 32611

MAY 15, 1996

PART I (Listings)

b. **Papers published in refereed journals**

1. J.-L. Calais, E. Deumens, and Y. Öhrn, "A Model for Electron Nuclear Dynamics of a Monatomic Chain" *J. Chem. Phys.* **101**, 3989 (1994)
2. R. Longo, B. Champagne, and Y. Öhrn, "Electron Propagator Theory and Application", *Theoretica Chimica Acta* **90**, 397 (1995).
3. J. Morales, A. Diz, E. Deumens, and Y. Öhrn, "Molecular Vibrational State Distributions in Collisions" *Chem. Phys. Lett.* **233**, 392 (1995).
4. A. Diz, Y. Öhrn, and J. R. Sabin, "Dynamic Charge States and Energy Deposition of Swift Helium Ions in Neon."*Nucl. Instr. Meth.***B96**, 633 (1995).
5. J. Morales, A. Diz, E. Deumens, and Y. Öhrn, "Electron nuclear dynamics of $H^+ + H_2$ collisions at E_{cm} = 20 eV.", *J. Chem. Phys.* **103**. 9968 (1995).
6. D. Beksic and D. A. Micha "Electronically Diabatic Quantum Dynamics of Molecular Desorption", *J. Chem. Phys.***103**, 3795–3808 (1995).

h. **Invited presentations**

1. Francqui Lecture (Y.Ö.) "Time and Chemistry", at F.U.N.D.P., Namur, Belgium, June 2, 1995.
2. Memorial Symposium for J.-L. Calais, at Uppsala University, Sweden, (Y. Ö.) "Electron Nuclear Dynamics", June 15, 1995.
3. Seminar (Y.Ö.) "Electron Nuclear Dynamics" at the University of Mons, Mons, Belgium, September 13, 1995.
4. Seminar (Y.Ö.) "Coherent States in Molecular Reactive Collisions" the University of Leuven, Belgium September 19, 1995.
5. Seminar (D. A. M.) "Quantum Dynamics of CO Photodissociation from the Ni(001) Surface", Chemistry Department, Univ. of Tennessee (Knoxville), Oct. 2, 1995.
6. Francqui Symposium (Y.Ö.) "Quantum Chemistry; An Overview and a Look to the Future", F. U. N. D. P. , Namur, Belgium October 27, 1995.

j. **Awards**

N. Yngve Öhrn was awarded the Francqui Professorship (Chaire Francqui Interuniversitaires au Titre Etranger) at Belgian Universities for 1995. This annual award is given in all areas of academe. Dr. Öhrn was the first chemist to receive this honor.

l. **Other funding**

National Science Foundation "Theoretical and Computational Methods of Quantum Molecular Dynamics", $ 227,800/(3 years); 2/1/93 to 31/1/96 (extended to 31/1/97); P.I.: D. A. Micha. This grant supports development of methodology and applications to molecular systems different from the ones in the present ONR Grant.

PART II

a. Principal Investigator; N. Yngve Öhrn; Co-principal Investigator: David A. Micha

b. Institute phone number: (352) 392–1597

c. Cognizant ONR Scientific Officer: Parbury P. Schmidt

d. **Description of the project**

This proposal concerns the development and application of theory and computational methods to the spectra and dynamics of molecules adsorbed on solid surfaces. The goals include (a) the development of theory of, in particular, photoelectron spectra and dynamics of adsorbed species with proper account of electronic-nuclear coupling and media effects and (b) the development of the quantum molecular dynamics of atoms and molecules at solid surfaces, and in particular photodesorption and electron transfer at surfaces. The methodologies include electron propagator theory, density matrix and coherent state formulations of quantum molecular dynamics, wavepacket propagation, and molecular dynamics simulations. The research provides information on the structure of adsorbates and helps elucidate mechanisms involved in reactions at solid surfaces, aiding the understanding of adhesion and surface bonding processes. It concerns molecular forces at interfaces, electronic excitation and electron transfer at surfaces, and temperature effects at solid surfaces.

g. **Names of research associates and students.**

Postdoctoral Research Associates: Keith Runge (100%); Benny Mogensen (50%); Anna Pohl (50%); Graduate Research Assistants: Jorge A. Morales (100%).